

What is claimed is:

1. A method for analyzing a complex biological sample using a Fourier Transform Mass Spectrometer (FTMS), said method comprising the steps of:

- a. ionizing a sample to produce sample (molecular) ions;
- b. introducing said ions into an analysis region of said FTMS;
- c. analyzing said ions to determine the molecular weight and abundance of said ions;
- d. utilizing said molecular weight to determine the empirical formula of each species of said sample; and
- e. identifying each said species by comparing said empirical formula to a database of formulas for known molecules.

2. A method according to claim 1, wherein said determining of the molecular weight is performed with an accuracy sufficient to identify empirical formula of said ions.

3. A method according to claim 1, wherein said database of known molecules is updated with said determined molecular structures.

4. A method for analyzing a complex biological sample using a Fourier Transform Mass Spectrometer (FTMS), said method comprising the steps of:

- a. ionizing a sample to produce sample (molecular) ions;
- b. introducing said ions into an analysis region of said FTMS;
- c. analyzing said ions to determine the molecular weight and abundance of said ions;
- d. determining the molecular structure of each species by multiple stages of mass spectrometry; and
- e. producing a profile of the sample showing structure and concentration data for each species.

5. A method according to claim 4, wherein said determining of the molecular weight is performed with an accuracy sufficient to identify empirical formula of said ions.

6. A method for analyzing a complex biological sample using a Fourier Transform Mass Spectrometer (FTMS), said method comprising the steps of:

- a. ionizing the sample to produce sample precursor ions;
- b. introducing said ions into the analysis region of said FTMS;
- c. analyzing said ions to determine the molecular weight, the abundance and the empirical formula of said ions;
- d. fragmenting said sample precursor ions to produce fragment ions;
- e. determining the molecular weight, the abundance and empirical formula of said fragment ions;
- f. determining the structure of said fragment ions by comparing said empirical formulas of said fragment ions to a database of fragments with known structure;
- g. combining said structures of said fragment ions to determine the precursor ion structure for each species in said sample; and
- h. producing a profile of said sample showing structure and concentration data for selected species of said sample.

7. A method according to claim 6, wherein said determining of the molecular weight is performed with an accuracy sufficient to identify empirical formula of said ions.

8. A method according to claim 6, wherein said fragmenting is performed using photodissociation.

9. A method for analyzing a complex biological sample utilizing Fourier Transform Mass Spectrometry (FTMS), said method comprising the steps of:

- a. ionizing polar molecules using positive and negative electrospray to produce sample (molecular) ions;
- b. introducing said ions into an analysis region of said FTMS;
- c. analyzing said ions to determine the molecular weight and abundance of said ions;
- d. utilizing said molecular weight to determine the empirical formula of each species of said sample; and
- e. identifying each said species by comparing said empirical formula to a database of formulas for known molecules.

10. A method according to claim 9, wherein said determining of the molecular weight is performed with an accuracy sufficient to identify empirical formula of said ions.

11. A method according to claim 9, wherein said database of known molecules is updated with said determined molecular structures.

12. A method for analyzing a complex biological sample utilizing Fourier Transform Mass Spectrometry (FTMS), said method comprising the steps of:

a. ionizing non-polar molecules using positive and negative ion atmospheric pressure chemical ionization to produce sample (molecular) ions.

b. introducing said ions into an analysis region of said FTMS;

c. analyzing said ions to determine the molecular weight and abundance of said ions;

d. utilizing said molecular weight to determine the empirical formula of each species of said sample; and

e. identifying each said species by comparing said empirical formula to a database of formulas for known molecules.

13. A method according to claim 12, wherein said determining of the molecular weight is performed with an accuracy sufficient to identify empirical formula of said ions.

5 14. A method according to claim 12, wherein said database of known molecules is updated with said determined molecular structures.